



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2026 – 05:57 PM EDT

PDB ID : 38LQ / pdb_000038lq
Title : Structure of Staphylococcus aureus Y131F DNA gyrase GK-del fusion construct in complex with 20 bp DNA and OSU-276
Authors : Tomaszewski, A.J.; Bell, C.E.
Deposited on : 2026-09-02
Resolution : 1.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

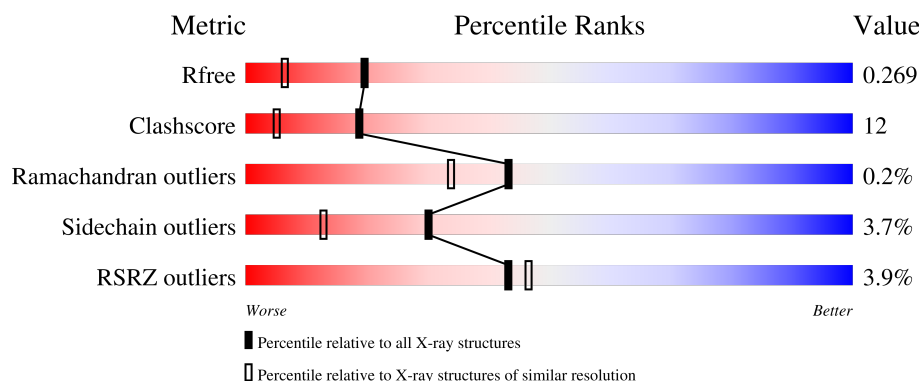
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	693	 4% 68% 25% . .
1	B	693	 4% 67% 27% . .
2	C	20	 40% 40% 20%
2	D	20	 35% 50% 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12471 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	3	0
			5331	3322	964	1020	25			
1	B	671	Total	C	N	O	S	0	3	0
			5343	3332	964	1022	25			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	GLY	-	expression tag	UNP P66936
A	409	MET	-	expression tag	UNP P66936
A	544	THR	-	linker	UNP P66936
A	545	GLY	-	linker	UNP P66936
A	1123	PHE	TYR	engineered mutation	UNP Q99XG5
B	408	GLY	-	expression tag	UNP P66936
B	409	MET	-	expression tag	UNP P66936
B	544	THR	-	linker	UNP P66936
B	545	GLY	-	linker	UNP P66936
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5

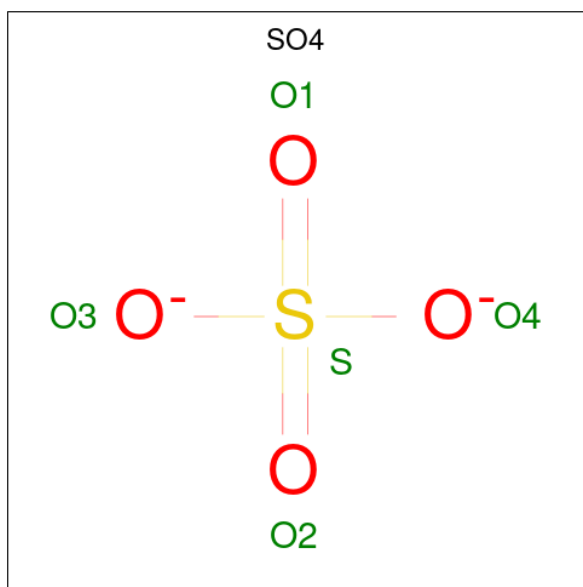
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			410	193	77	120	20			
2	D	20	Total	C	N	O	P	0	0	0
			390	183	75	113	19			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

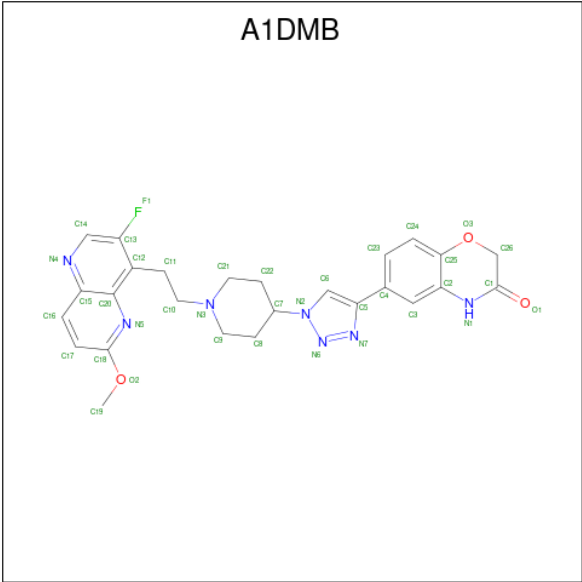
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is (6P)-6-(1-{1-[2-(3-fluoro-6-methoxy-1,5-naphthyridin-4-yl)ethyl]piperidin-4-yl}-1H-1,2,3-triazol-4-yl)-2H-1,4-benzoxazin-3(4H)-one (CCD ID: A1DMB) (formula: C₂₆H₂₆FN₇O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	F	N	O	0	0
			37	26	1	7	3		

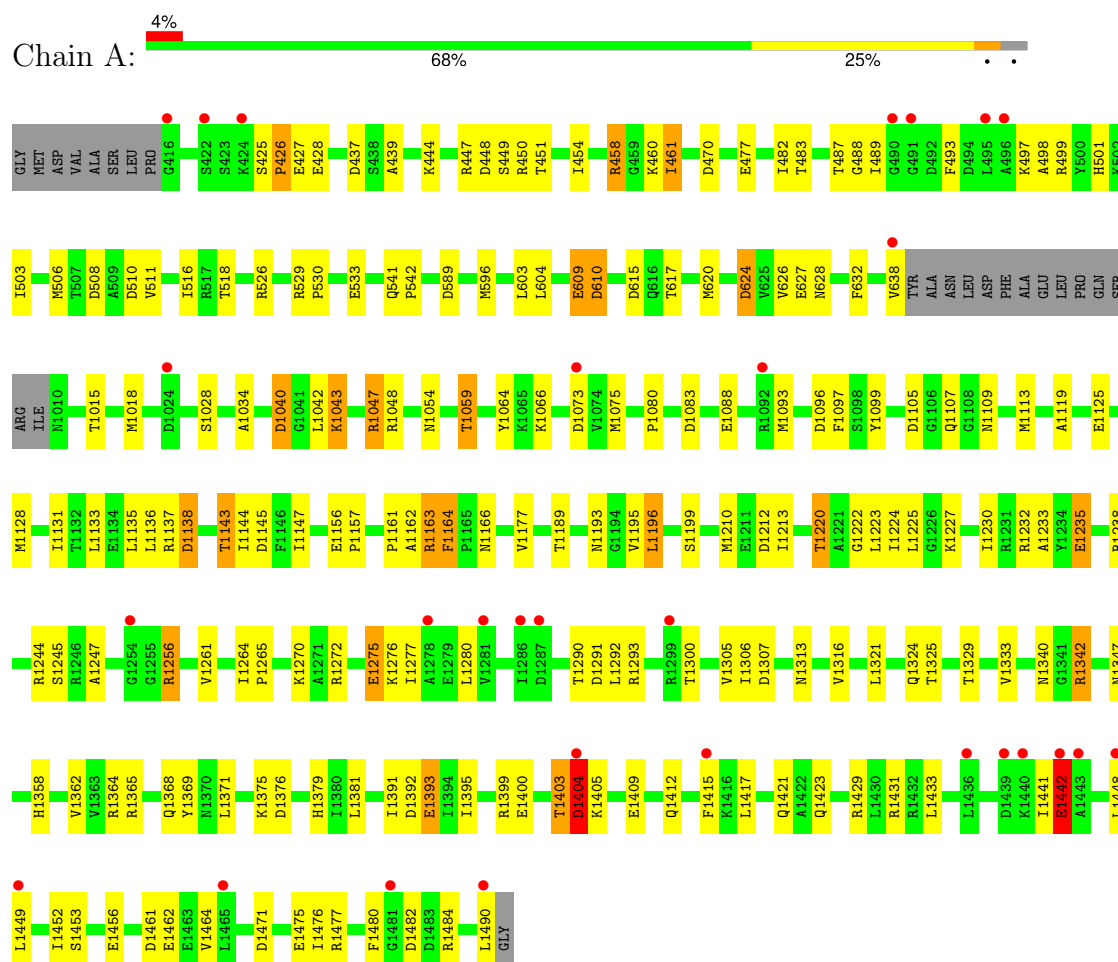
- Molecule 6 is water.

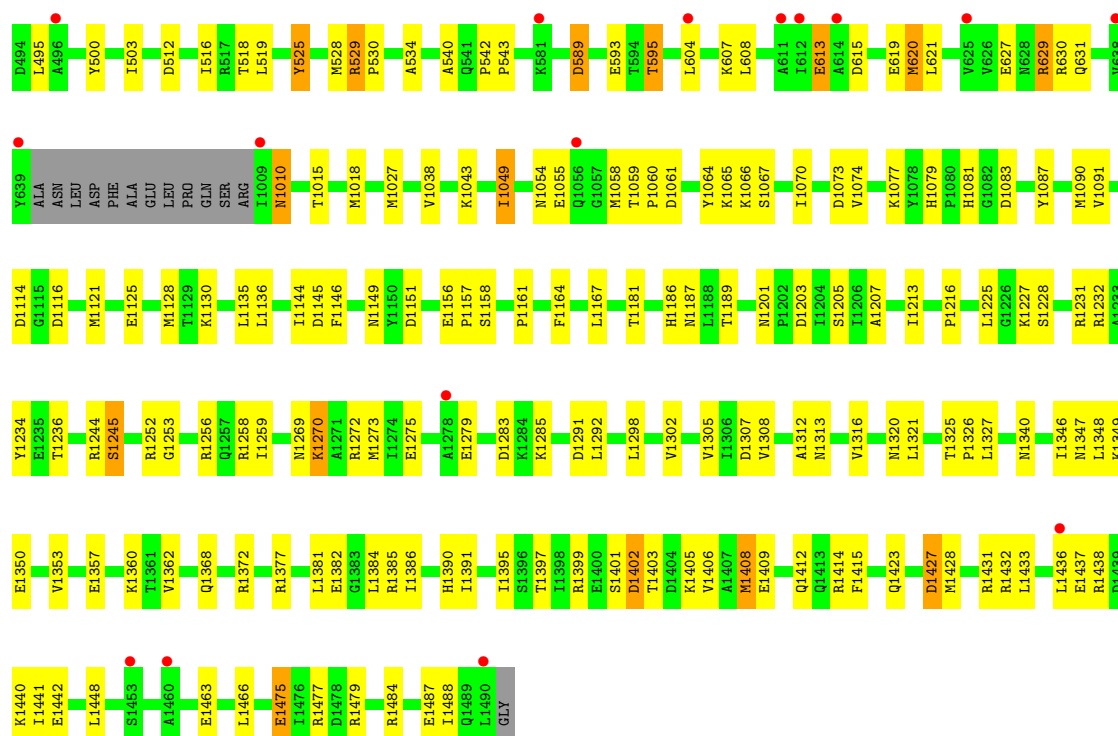
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	387	Total	O	0	0
			387	387		
6	B	423	Total	O	0	0
			423	423		
6	C	55	Total	O	0	0
			55	55		
6	D	63	Total	O	0	0
			63	63		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

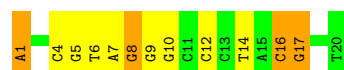
- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A





● Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*C
P*GP*GP*CP*T)-3')

Chain C: 40% 40% 20%



● Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*C
P*GP*GP*CP*T)-3')

Chain D: 35% 50% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.72Å 92.72Å 402.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.30 – 1.84 80.30 – 1.84	Depositor EDS
% Data completeness (in resolution range)	69.5 (80.30-1.84) 70.9 (80.30-1.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.169 , 0.238 0.192 , 0.269	Depositor DCC
R_{free} test set	6308 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.715 for H, K, L 0.285 for -K, -H, -L	Depositor
Outliers	0 of 120174 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12471	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MN, A1DMB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/5402	1.42	46/7274 (0.6%)
1	B	0.69	0/5415	1.41	32/7294 (0.4%)
2	C	1.15	1/459 (0.2%)	1.84	17/706 (2.4%)
2	D	1.18	0/437	1.86	11/674 (1.6%)
All	All	0.74	1/11713 (0.0%)	1.46	106/15948 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DA	P-O5'	8.32	1.68	1.59

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	DG	O4'-C4'-C3'	-11.13	99.32	106.00
1	B	1203	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	1146	PHE	CA-CB-CG	-7.78	106.03	113.80
2	C	8	DG	C4'-C3'-C2'	-7.65	96.22	103.10
1	A	458	ARG	CB-CA-C	-7.60	99.65	111.74
1	A	1393	GLU	CB-CG-CD	7.31	125.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	17	DG	O4'-C1'-N9	-7.24	102.93	108.00
2	D	14	DT	O4'-C4'-C3'	-7.19	101.68	106.00
2	C	4	DC	O5'-C5'-C4'	-6.91	103.87	109.40
1	A	470	ASP	CA-CB-CG	6.88	119.48	112.60
1	B	525	TYR	N-CA-CB	6.78	120.13	109.82
1	B	1216	PRO	CB-CA-C	6.75	119.79	110.95
1	A	1105	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	1093	MET	CG-SD-CE	-6.70	86.16	100.90
1	B	589	ASP	CA-CB-CG	6.60	119.20	112.60
2	C	9	DG	C4'-C3'-C2'	-6.58	97.18	103.10
1	A	1138	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	1073	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	1471	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	506	MET	CG-SD-CE	6.33	114.83	100.90
1	B	629	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	B	1213	ILE	N-CA-CB	-6.25	105.39	111.89
1	B	1475	GLU	CB-CG-CD	6.23	123.19	112.60
2	D	17	DG	O4'-C1'-N9	-6.21	103.65	108.00
2	C	1	DA	C4'-C3'-C2'	-6.21	97.51	103.10
2	C	1	DA	O4'-C4'-C3'	-6.19	102.29	106.00
2	D	7	DA	O4'-C4'-C3'	-6.19	102.29	106.00
1	A	1096	ASP	CB-CA-C	5.99	120.79	110.01
1	A	1235	GLU	N-CA-CB	5.95	119.47	110.30
1	B	1350	GLU	N-CA-CB	5.95	118.64	110.01
1	A	617	THR	CA-CB-OG1	-5.95	100.68	109.60
2	C	7	DA	C4'-C3'-C2'	-5.92	97.77	103.10
1	B	1436	LEU	N-CA-CB	5.92	118.82	110.12
1	B	1415	PHE	CA-CB-CG	-5.91	107.89	113.80
1	B	1116	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	1376	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	1427	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	1402	ASP	CB-CA-C	-5.79	101.55	110.81
1	B	1151	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	1342	ARG	CB-CA-C	-5.75	99.95	109.15
1	B	593	GLU	CB-CG-CD	5.74	122.35	112.60
1	B	1236	THR	CA-CB-OG1	-5.72	101.01	109.60
1	B	619	GLU	CB-CG-CD	5.71	122.31	112.60
2	C	16	DC	C1'-O4'-C4'	-5.71	104.39	110.10
1	A	1482	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	615	ASP	CA-CB-CG	5.70	118.30	112.60
2	C	12	DC	O4'-C1'-N1	5.67	111.97	108.00
1	B	615	ASP	CA-CB-CG	5.66	118.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1390	HIS	CB-CA-C	-5.66	100.70	111.97
1	B	1181	THR	CA-CB-OG1	-5.65	101.13	109.60
1	A	448	ASP	CA-CB-CG	5.63	118.23	112.60
2	D	12	DC	O4'-C1'-N1	5.63	111.94	108.00
1	A	1369	TYR	N-CA-CB	5.62	118.21	110.07
2	C	16	DC	O4'-C4'-C3'	-5.61	102.64	106.00
1	A	589	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	1040	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	1196	LEU	CA-C-N	5.51	127.94	120.44
1	A	1196	LEU	C-N-CA	5.51	127.94	120.44
1	A	1043	LYS	CB-CA-C	5.51	118.14	109.37
1	A	1272	ARG	CB-CA-C	5.51	119.93	110.79
1	A	1276	LYS	N-CA-CB	5.49	118.19	110.12
1	A	1329	THR	OG1-CB-CG2	-5.47	98.35	109.30
1	B	1340	ASN	CB-CA-C	5.47	119.79	111.80
1	A	1195	VAL	N-CA-CB	5.46	117.96	110.54
2	D	5	DG	O4'-C1'-N9	5.45	111.81	108.00
1	B	525	TYR	CB-CA-C	-5.44	102.27	110.92
1	A	1161	PRO	CB-CA-C	5.43	122.10	112.64
2	D	19	DC	C1'-O4'-C4'	-5.43	104.67	110.10
1	B	487	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	1193	ASN	CB-CA-C	5.42	119.49	110.81
1	A	1409	GLU	CB-CA-C	-5.42	102.61	110.96
2	C	16	DC	O5'-C5'-C4'	-5.38	105.09	109.40
1	B	1049	ILE	N-CA-C	-5.35	105.50	110.53
1	B	1292	LEU	N-CA-CB	-5.34	101.50	110.32
2	C	6	DT	P-O3'-C3'	5.34	126.11	119.70
1	A	1096	ASP	CA-CB-CG	5.33	117.93	112.60
2	D	4	DC	O4'-C4'-C3'	-5.33	102.80	106.00
1	B	1347	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	1462	GLU	CB-CA-C	-5.32	101.90	110.74
2	D	11	DC	N1-C2-O2	5.29	122.08	118.90
1	B	1079	HIS	CB-CA-C	5.28	119.10	111.02
2	D	10	DG	O4'-C4'-C3'	5.26	109.16	106.00
1	A	508	ASP	CA-CB-CG	5.25	117.85	112.60
2	C	1	DA	O4'-C1'-N9	5.21	111.65	108.00
1	A	483	THR	CA-CB-OG1	-5.21	101.79	109.60
1	B	1477	ARG	CB-CA-C	-5.21	102.70	110.88
2	D	16	DC	C1'-O4'-C4'	-5.20	104.90	110.10
1	A	1212	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	1099	TYR	CB-CA-C	5.18	118.29	109.75
2	C	8	DG	P-O3'-C3'	5.17	125.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	DA	O5'-C5'-C4'	-5.15	105.28	109.40
1	A	1393	GLU	CB-CA-C	5.15	120.55	110.67
1	A	1275	GLU	CB-CA-C	5.13	119.30	110.79
1	A	1080	PRO	N-CA-CB	-5.12	98.66	102.25
1	A	1015	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	1404	ASP	CB-CA-C	5.12	117.57	111.22
2	D	10	DG	P-O3'-C3'	5.11	125.84	119.70
1	B	1055	GLU	CB-CA-C	-5.11	102.16	110.85
1	B	1357	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	439	ALA	CA-C-N	5.10	125.64	119.98
1	A	439	ALA	C-N-CA	5.10	125.64	119.98
1	A	1047	ARG	CD-NE-CZ	5.08	131.50	124.40
1	B	1186	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	1442	GLU	N-CA-CB	5.04	117.53	110.12
1	A	1164	PHE	CA-CB-CG	5.01	118.81	113.80
2	C	14	DT	C4'-C3'-C2'	-5.01	98.59	103.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	ARG	Sidechain
1	A	1163	ARG	Sidechain
1	A	1256	ARG	Sidechain
1	A	1399	ARG	Sidechain
1	A	499	ARG	Sidechain
1	B	1385	ARG	Sidechain
1	B	1479	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5331	0	5388	124	0
1	B	5343	0	5397	144	0
2	C	410	0	224	7	0
2	D	390	0	209	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
5	C	37	0	0	0	0
6	A	387	0	0	19	3
6	B	423	0	0	31	2
6	C	55	0	0	3	1
6	D	63	0	0	3	0
All	All	12471	0	11218	271	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (271) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:LEU:O	1:A:1325:THR:OG1	1.88	0.92
1:B:1484:ARG:O	6:B:1601:HOH:O	1.93	0.84
1:B:1273:MET:HG3	1:B:1326:PRO:HG2	1.63	0.81
1:B:1207:ALA:HB2	1:B:1231[B]:ARG:NH2	1.96	0.80
1:A:1147:ILE:HG22	6:A:1944:HOH:O	1.82	0.80
1:B:631:GLN:OE1	6:B:1602:HOH:O	2.03	0.76
1:B:476:ASN:HB2	6:B:1694:HOH:O	1.86	0.76
1:A:1423:GLN:OE1	1:B:1431:ARG:NH1	2.18	0.75
1:B:627:GLU:OE2	6:B:1602:HOH:O	2.05	0.75
1:A:1449:LEU:O	6:A:1601:HOH:O	2.06	0.74
1:B:1256:ARG:NH1	6:B:1609:HOH:O	2.17	0.73
1:A:1088:GLU:CD	6:A:1639:HOH:O	2.32	0.71
1:B:1438:ARG:O	6:B:1603:HOH:O	2.09	0.71
1:B:1360:LYS:HD2	1:B:1466:LEU:HD13	1.73	0.71
1:B:1272:ARG:NH2	6:B:1613:HOH:O	2.24	0.70
1:B:1405:LYS:O	1:B:1409:GLU:HG3	1.92	0.69
1:A:1431:ARG:NH2	1:B:1423:GLN:OE1	2.20	0.69
1:A:1490:LEU:O	6:A:1602:HOH:O	2.10	0.69
1:B:464:VAL:HG12	1:B:472:ILE:HG12	1.75	0.69
2:C:1:DA:N3	2:C:1:DA:H5'	2.09	0.68
1:B:589:ASP:OD1	6:B:1604:HOH:O	2.12	0.67
1:B:1058:MET:HE2	1:B:1065:LYS:HG3	1.74	0.67
6:B:1612:HOH:O	2:D:10:DG:N3	2.28	0.66
1:A:501:HIS:O	6:A:1603:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1487:GLU:OE1	6:B:1605:HOH:O	2.12	0.66
1:B:1427:ASP:OD2	6:B:1606:HOH:O	2.14	0.65
1:A:1196:LEU:O	1:A:1199:SER:OG	2.14	0.65
1:B:1302:VAL:O	6:B:1607:HOH:O	2.14	0.65
1:A:501:HIS:ND1	6:A:1612:HOH:O	2.24	0.65
1:B:1232:ARG:NH1	6:B:1624:HOH:O	2.29	0.65
1:B:1225:LEU:HD11	1:B:1244:ARG:HG3	1.79	0.64
1:B:1207:ALA:HB2	1:B:1231[B]:ARG:HH22	1.61	0.64
1:A:497:LYS:O	1:A:498:ALA:C	2.39	0.64
1:B:450:ARG:HB3	1:B:451:THR:HG23	1.79	0.64
1:B:1144:ILE:C	1:B:1144:ILE:HD12	2.23	0.64
1:A:1429:ARG:NH1	1:B:1427:ASP:O	2.31	0.63
1:B:1227:LYS:HE2	1:B:1488:ILE:HG21	1.79	0.63
1:B:1273:MET:CG	1:B:1326:PRO:HG2	2.29	0.63
1:A:1392:ASP:OD2	1:B:1399:ARG:NH1	2.31	0.63
1:A:1144:ILE:HD12	1:A:1144:ILE:O	2.00	0.62
1:A:1280:LEU:HD22	1:A:1324:GLN:NE2	2.15	0.62
1:A:1364:ARG:O	1:A:1368:GLN:HG3	1.98	0.62
1:A:1291:ASP:OD1	1:A:1292:LEU:N	2.32	0.62
1:B:444:LYS:HA	1:B:454:ILE:CD1	2.30	0.62
1:A:1475:GLU:OE1	6:A:1604:HOH:O	2.16	0.62
1:B:1073:ASP:OD1	1:B:1077:LYS:NZ	2.32	0.62
1:B:1043:LYS:NZ	6:B:1625:HOH:O	2.30	0.61
1:B:433:LEU:HD23	1:B:455:LEU:HB3	1.81	0.61
1:A:1461:ASP:O	1:A:1464:VAL:HG12	2.00	0.61
2:D:1:DA:O4'	2:D:1:DA:N3	2.31	0.61
1:B:1070:ILE:O	1:B:1074:VAL:HG23	2.01	0.61
1:A:1144:ILE:O	6:A:1605:HOH:O	2.16	0.60
2:D:5:DG:O4'	6:D:102:HOH:O	2.17	0.60
1:A:1342:ARG:HG3	1:A:1342:ARG:HH21	1.67	0.60
2:D:15:DA:OP2	6:D:101:HOH:O	2.16	0.60
1:A:1381:LEU:HD22	1:A:1441:ILE:HG23	1.82	0.59
1:A:1144:ILE:HD12	1:A:1144:ILE:C	2.27	0.59
1:B:518:THR:HB	1:B:1018:MET:HE1	1.84	0.59
1:B:1298:LEU:HD23	6:B:1931:HOH:O	2.02	0.59
1:A:1075:MET:HE1	1:A:1083:ASP:HB3	1.85	0.59
1:A:1227:LYS:HE3	6:A:1920:HOH:O	2.03	0.58
1:A:1313:ASN:CG	1:A:1316:VAL:HG23	2.28	0.58
1:B:1083:ASP:HB2	1:B:1121:MET:HE1	1.85	0.58
1:B:1059:THR:OG1	1:B:1061:ASP:OD1	2.16	0.58
1:A:1393:GLU:HG3	1:A:1415:PHE:HZ	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:LEU:HD21	1:A:1244:ARG:HD2	1.85	0.57
1:A:444[A]:LYS:HA	1:A:454:ILE:CD1	2.34	0.57
1:A:1247:ALA:HB2	1:A:1261:VAL:HG22	1.86	0.57
1:A:1442:GLU:OE1	1:A:1442:GLU:HA	2.04	0.57
1:A:437:ASP:HB2	2:C:10:DG:H5"	1.85	0.57
1:A:1452:ILE:HG22	1:A:1456:GLU:OE2	2.04	0.57
1:A:1358:HIS:O	1:A:1362:VAL:HG23	2.05	0.57
1:B:1073:ASP:OD1	1:B:1077:LYS:CE	2.54	0.56
1:B:1253:GLY:O	6:B:1610:HOH:O	2.18	0.56
1:B:529:ARG:N	1:B:530:PRO:CD	2.68	0.56
1:A:447:ARG:HD3	1:A:454:ILE:HD11	1.87	0.56
1:B:1382:GLU:O	1:B:1386:ILE:HG13	2.06	0.56
2:C:17:DG:N7	6:C:201:HOH:O	2.33	0.55
1:A:1404:ASP:OD1	1:A:1404:ASP:N	2.37	0.55
1:A:461:ILE:HG22	6:A:1788:HOH:O	2.05	0.55
1:A:1280:LEU:CD2	1:A:1324:GLN:HE21	2.19	0.55
1:B:493:PHE:CE1	1:B:530:PRO:HB2	2.42	0.55
1:A:1379:HIS:O	1:A:1421:GLN:NE2	2.24	0.55
1:B:529:ARG:N	1:B:530:PRO:HD2	2.22	0.55
1:B:1256:ARG:NH1	6:B:1644:HOH:O	2.40	0.55
1:B:1320:ASN:ND2	6:B:1643:HOH:O	2.40	0.54
1:A:1245:SER:OG	1:A:1265:PRO:HD3	2.07	0.54
1:B:1258:ARG:HD2	1:B:1305:VAL:HG13	1.88	0.54
1:B:458:ARG:NH2	6:B:1612:HOH:O	2.24	0.54
1:B:1187:ASN:OD1	1:B:1189:THR:HB	2.07	0.54
1:B:1058:MET:HG2	1:B:1065:LYS:HG3	1.90	0.54
1:B:1402:ASP:HB2	1:B:1403:THR:HG23	1.90	0.54
1:B:620:MET:O	1:B:620:MET:HG2	2.07	0.54
1:B:1402:ASP:HA	6:B:1652:HOH:O	2.07	0.54
1:A:1034:ALA:O	1:A:1043:LYS:HE2	2.08	0.54
1:B:1058:MET:HG2	1:B:1065:LYS:CE	2.38	0.53
1:B:1245:SER:OG	1:B:1327:LEU:HD12	2.08	0.53
1:A:626:VAL:O	1:A:627:GLU:C	2.49	0.53
1:A:1233:ALA:HB1	1:A:1333:VAL:HG11	1.90	0.53
1:A:1391:ILE:O	1:A:1395:ILE:HG12	2.08	0.53
1:A:1280:LEU:HD22	1:A:1324:GLN:HE21	1.73	0.53
1:B:630:ARG:NH2	6:B:1645:HOH:O	2.41	0.53
1:B:477:GLU:O	1:B:481:MET:HG3	2.09	0.53
1:B:604:LEU:HD23	1:B:1010:ASN:HB2	1.91	0.52
1:A:1224:ILE:HG21	1:A:1230:ILE:HD11	1.90	0.52
1:A:1131:ILE:HG12	1:A:1164:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:ARG:HG2	6:D:137:HOH:O	2.08	0.52
1:A:493:PHE:CE1	1:A:530:PRO:HB2	2.45	0.52
1:B:1256:ARG:NH2	6:B:1609:HOH:O	2.41	0.52
1:A:1393:GLU:HG3	1:A:1415:PHE:CZ	2.44	0.52
1:B:528:MET:C	1:B:530:PRO:HD2	2.34	0.52
1:B:1397:THR:O	1:B:1401:SER:OG	2.23	0.52
1:A:444[B]:LYS:HA	1:A:454:ILE:CD1	2.40	0.52
1:A:1097:PHE:HB3	1:A:1113:MET:HE3	1.92	0.51
1:B:1049:ILE:HD13	1:B:1090:MET:HB2	1.93	0.51
1:A:1232:ARG:HD3	6:A:1951:HOH:O	2.11	0.51
1:B:1252:ARG:HD3	1:B:1258:ARG:HB3	1.92	0.51
1:B:1384:LEU:HD22	1:B:1428:MET:HE2	1.92	0.51
1:B:444:LYS:HA	1:B:454:ILE:HD11	1.92	0.51
1:B:1067:SER:HB3	1:B:1090:MET:HE1	1.93	0.51
1:A:1113:MET:HE2	1:A:1220:THR:HG22	1.93	0.51
6:A:1940:HOH:O	1:B:1066:LYS:HB3	2.10	0.50
1:B:1234:TYR:CG	1:B:1348:LEU:HD22	2.46	0.50
1:A:487:THR:O	1:A:493:PHE:HA	2.11	0.50
1:A:1145:ASP:OD1	1:A:1365:ARG:NH1	2.32	0.50
1:B:525:TYR:O	1:B:529:ARG:HB2	2.12	0.50
1:A:1138:ASP:O	1:A:1143:THR:OG1	2.22	0.50
1:A:427:GLU:OE2	1:A:427:GLU:N	2.38	0.49
1:A:1292:LEU:CD1	1:A:1306:ILE:HG12	2.42	0.49
1:B:1010:ASN:HA	6:B:1926:HOH:O	2.11	0.49
1:A:460:LYS:HG2	2:C:8:DG:H1'	1.95	0.49
1:A:526:ARG:HB2	6:A:1875:HOH:O	2.12	0.49
1:B:1325:THR:HB	1:B:1326:PRO:HD2	1.95	0.49
1:B:1256:ARG:CZ	6:B:1609:HOH:O	2.60	0.49
1:A:1109:ASN:HB3	1:A:1119:ALA:HB2	1.95	0.48
1:B:1058:MET:CE	1:B:1065:LYS:HG3	2.42	0.48
1:B:529:ARG:HD3	1:B:608:LEU:CD2	2.43	0.48
1:B:1408:MET:HG3	1:B:1423:GLN:NE2	2.28	0.48
1:A:1290:THR:O	1:A:1291:ASP:CB	2.61	0.48
1:A:1461:ASP:HB3	1:A:1464:VAL:HG12	1.94	0.48
1:B:1144:ILE:HD12	1:B:1144:ILE:O	2.13	0.48
1:A:1391:ILE:HD13	1:A:1433:LEU:HD21	1.95	0.48
1:A:1412:GLN:HG2	1:A:1417:LEU:O	2.13	0.48
1:A:482:ILE:HD13	1:A:489:ILE:HD13	1.94	0.48
1:A:1059:THR:HG22	1:A:1133:LEU:HD21	1.96	0.48
1:B:1087:TYR:O	1:B:1091:VAL:HG23	2.14	0.48
1:A:1480:PHE:O	6:A:1606:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1275:GLU:HB2	6:A:1882:HOH:O	2.13	0.47
1:B:1058:MET:HG2	1:B:1065:LYS:CG	2.43	0.47
1:B:1408:MET:O	1:B:1412:GLN:HG3	2.14	0.47
1:A:428:GLU:O	1:A:451:THR:HB	2.14	0.47
1:B:1377:ARG:HB3	1:B:1448:LEU:HD21	1.97	0.47
1:A:427:GLU:HA	1:A:501:HIS:ND1	2.30	0.47
1:A:458:ARG:NE	6:A:1648:HOH:O	2.46	0.47
1:A:1484:ARG:NH1	1:A:1484:ARG:HG3	2.29	0.47
1:B:460:LYS:HA	1:B:516:ILE:HG12	1.95	0.47
1:B:1313:ASN:CG	1:B:1316:VAL:HG23	2.39	0.47
1:B:1081:HIS:HD2	2:D:8:DG:OP1	1.97	0.46
1:A:511:VAL:HG11	1:A:1028:SER:HB2	1.97	0.46
1:A:1066:LYS:NZ	1:A:1125:GLU:OE2	2.48	0.46
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	1.98	0.46
1:B:1440:LYS:HG3	6:B:1782:HOH:O	2.14	0.46
1:B:1081:HIS:HE1	6:B:1943:HOH:O	1.97	0.46
1:A:1135:LEU:HD23	1:A:1162:ALA:HA	1.96	0.46
1:A:1340:ASN:O	1:A:1342:ARG:NH2	2.49	0.46
1:B:447:ARG:NE	6:B:1647:HOH:O	2.42	0.46
1:A:620:MET:HE2	1:A:632:PHE:HB2	1.97	0.46
1:A:1107:GLN:HB3	1:A:1125:GLU:HB2	1.97	0.46
1:A:1177:VAL:HG22	2:D:16:DC:H4'	1.98	0.46
1:B:495:LEU:HD21	1:B:534:ALA:CB	2.46	0.46
1:B:1397:THR:HG23	1:B:1414:ARG:NH2	2.31	0.46
1:A:488:GLY:C	1:A:489:ILE:HG23	2.42	0.45
1:B:1114:ASP:OD1	1:B:1270:LYS:HB3	2.16	0.45
1:A:460:LYS:HD3	1:A:516:ILE:HG13	1.97	0.45
1:A:1347:ASN:OD1	1:A:1347:ASN:C	2.60	0.45
1:B:460:LYS:HD3	1:B:516:ILE:CG1	2.47	0.45
1:B:529:ARG:HD3	1:B:608:LEU:HD22	1.97	0.45
1:B:421:CYS:HB2	1:B:450:ARG:O	2.16	0.45
1:B:1273:MET:SD	1:B:1327:LEU:HD13	2.57	0.45
1:A:1163:ARG:O	1:A:1476:ILE:HD13	2.16	0.45
1:A:1371:LEU:HD11	1:A:1375:LYS:HE3	1.98	0.45
1:B:418:LEU:HB2	1:B:455:LEU:HD13	1.98	0.45
1:B:421:CYS:SG	1:B:429:CYS:SG	3.08	0.45
1:B:1135:LEU:HG	1:B:1164:PHE:CE1	2.51	0.45
1:B:1433:LEU:O	1:B:1438:ARG:HD3	2.15	0.45
1:A:541:GLN:NE2	1:A:604:LEU:HG	2.31	0.45
1:B:1269:ASN:HB3	1:B:1272:ARG:HB2	1.99	0.45
1:A:1290:THR:O	1:A:1291:ASP:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:HD13	1:A:1047:ARG:HA	2.00	0.44
1:B:540:ALA:HB1	1:B:595:THR:HG22	1.99	0.44
1:B:1368:GLN:O	1:B:1372:ARG:HG3	2.18	0.44
1:A:542:PRO:HD2	6:A:1907:HOH:O	2.18	0.44
1:A:530:PRO:HA	1:A:533:GLU:HB2	2.00	0.44
1:B:460:LYS:HD3	1:B:516:ILE:HG13	1.99	0.44
1:B:1475:GLU:HB2	6:B:1976:HOH:O	2.17	0.44
1:B:1058:MET:SD	1:B:1065:LYS:HG3	2.57	0.44
1:B:1308:VAL:CG1	1:B:1312:ALA:HB3	2.47	0.44
1:B:1073:ASP:OD1	1:B:1077:LYS:HE3	2.18	0.44
1:A:458:ARG:NH2	2:C:10:DG:H1'	2.33	0.44
1:A:510:ASP:OD2	6:A:1607:HOH:O	2.21	0.44
1:B:621:LEU:O	1:B:629:ARG:HD3	2.18	0.44
1:B:1058:MET:HG2	1:B:1065:LYS:HE3	2.00	0.44
1:B:1283:ASP:O	1:B:1285:LYS:HG3	2.18	0.44
1:B:1401:SER:HB3	1:B:1406:VAL:HG12	1.99	0.44
1:B:1059:THR:HB	1:B:1060:PRO:CD	2.48	0.44
1:B:1054:ASN:HA	1:B:1128:MET:CE	2.48	0.43
1:B:1205:SER:HA	6:B:1783:HOH:O	2.18	0.43
1:B:1234:TYR:CD2	1:B:1348:LEU:HD22	2.53	0.43
1:B:1273:MET:HE2	1:B:1273:MET:HB3	1.89	0.43
1:A:444[A]:LYS:HA	1:A:454:ILE:HD11	1.99	0.43
1:B:1149:ASN:OD1	1:B:1149:ASN:C	2.61	0.43
1:A:1222:GLY:C	1:A:1223:LEU:HD12	2.43	0.43
1:B:516:ILE:HA	1:B:519:LEU:HD12	2.00	0.43
2:C:16:DC:H1'	6:C:205:HOH:O	2.17	0.43
1:B:613:GLU:HG3	1:B:1015:THR:HG21	1.99	0.43
1:B:1321:LEU:O	1:B:1325:THR:OG1	2.34	0.43
1:A:1293:ARG:NH1	1:A:1307:ASP:OD2	2.41	0.43
1:A:1210:MET:HA	1:A:1213:ILE:O	2.19	0.43
1:A:1264:ILE:HD13	1:A:1270:LYS:HB2	2.01	0.43
1:B:1391:ILE:O	1:B:1395:ILE:HG12	2.18	0.43
1:A:1137:ARG:HD2	6:A:1914:HOH:O	2.19	0.43
1:A:1342:ARG:HG3	1:A:1342:ARG:NH2	2.32	0.43
1:B:420:ASP:OD1	1:B:500:TYR:OH	2.29	0.43
1:B:469:LEU:HA	1:B:472:ILE:HD12	2.01	0.43
1:B:1432:ARG:NH2	6:B:1658:HOH:O	2.50	0.43
1:B:1038:VAL:HA	1:B:1167:LEU:HD22	2.00	0.43
1:B:421:CYS:HG	1:B:429:CYS:HG	1.56	0.42
1:A:1040:ASP:O	1:A:1166:ASN:HB3	2.19	0.42
1:A:1293:ARG:NH2	1:A:1305:VAL:HG11	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:ASP:O	1:B:493:PHE:C	2.62	0.42
1:B:512:ASP:O	1:B:516:ILE:HD12	2.19	0.42
1:B:1442:GLU:HB2	6:B:1603:HOH:O	2.19	0.42
1:B:1054:ASN:HB2	1:B:1136:LEU:HD13	2.01	0.42
1:B:1291:ASP:HB3	1:B:1307:ASP:HB2	2.01	0.42
1:A:1064:TYR:HB3	1:A:1125:GLU:HB3	2.00	0.42
1:B:444:LYS:HG3	1:B:454:ILE:HD12	2.02	0.42
1:B:1156:GLU:HB2	1:B:1157:PRO:HD2	2.01	0.42
1:B:1408:MET:SD	1:B:1423:GLN:NE2	2.93	0.42
1:B:1201:ASN:OD1	1:B:1201:ASN:C	2.62	0.42
1:B:1349:LYS:O	1:B:1353:VAL:HG23	2.19	0.42
1:B:1463:GLU:O	1:B:1463:GLU:HG3	2.17	0.42
1:A:1054:ASN:HA	1:A:1128:MET:HE2	2.02	0.42
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.93	0.42
1:B:495:LEU:HD21	1:B:534:ALA:HB2	2.02	0.41
1:B:1145:ASP:O	1:B:1158:SER:OG	2.35	0.41
1:A:447:ARG:HB3	1:A:596:MET:HE1	2.03	0.41
1:A:609:GLU:O	1:A:610:ASP:HB2	2.20	0.41
1:A:1448:LEU:HD23	1:A:1448:LEU:HA	1.98	0.41
1:A:626:VAL:O	1:A:628:ASN:N	2.53	0.41
1:A:1144:ILE:C	1:A:1144:ILE:CD1	2.92	0.41
1:A:529:ARG:N	1:A:530:PRO:CD	2.83	0.41
1:A:1277:ILE:HG13	1:A:1325:THR:HG21	2.03	0.41
1:A:518:THR:HB	1:A:1018:MET:HE1	2.03	0.41
1:A:1054:ASN:HB2	1:A:1136:LEU:HD13	2.02	0.41
1:B:1437:GLU:OE2	1:B:1437:GLU:HA	2.21	0.41
1:A:425:SER:O	1:A:426:PRO:C	2.62	0.41
1:A:1256:ARG:NH1	4:A:1503:SO4:O3	2.53	0.41
1:A:450[B]:ARG:CZ	1:A:451:THR:CG2	2.98	0.41
1:A:482:ILE:CD1	1:A:489:ILE:HD13	2.51	0.41
1:A:1054:ASN:HA	1:A:1128:MET:CE	2.50	0.41
1:A:1403:THR:C	1:A:1405:LYS:H	2.28	0.41
1:B:448:ASP:OD1	1:B:448:ASP:C	2.64	0.41
2:C:5:DG:H8	6:C:210:HOH:O	2.03	0.41
1:B:1059:THR:HB	1:B:1060:PRO:HD2	2.03	0.41
1:B:1245:SER:OG	1:B:1327:LEU:CD1	2.68	0.41
1:B:1381:LEU:HD22	1:B:1441:ILE:HG23	2.02	0.40
1:A:1189:THR:HA	1:A:1477:ARG:HG3	2.03	0.40
1:A:1391:ILE:CD1	1:A:1433:LEU:HD21	2.51	0.40
1:A:1156:GLU:HB2	1:A:1157:PRO:HD2	2.03	0.40
1:A:624:ASP:OD1	1:A:624:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:ASN:ND2	1:B:441:GLY:HA3	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1930:HOH:O	6:C:240:HOH:O[1_565]	2.01	0.19
6:A:1819:HOH:O	6:B:1970:HOH:O[6_555]	2.07	0.13
6:A:1972:HOH:O	6:B:1927:HOH:O[1_665]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	669/693 (96%)	635 (95%)	33 (5%)	1 (0%)	48	38
1	B	670/693 (97%)	632 (94%)	37 (6%)	1 (0%)	48	38
All	All	1339/1386 (97%)	1267 (95%)	70 (5%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	610	ASP
1	B	1245	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/591 (98%)	557 (97%)	19 (3%)	33	15
1	B	577/591 (98%)	553 (96%)	24 (4%)	26	8
All	All	1153/1182 (98%)	1110 (96%)	43 (4%)	30	13

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	426	PRO
1	A	449	SER
1	A	461	ILE
1	A	477	GLU
1	A	503	ILE
1	A	603	LEU
1	A	609	GLU
1	A	624	ASP
1	A	638	VAL
1	A	1059	THR
1	A	1143	THR
1	A	1220	THR
1	A	1235	GLU
1	A	1300	THR
1	A	1400	GLU
1	A	1403	THR
1	A	1404	ASP
1	A	1442	GLU
1	A	1453	SER
1	B	418	LEU
1	B	422	SER
1	B	424	LYS
1	B	449	SER
1	B	477	GLU
1	B	503	ILE
1	B	529	ARG
1	B	595	THR
1	B	607	LYS
1	B	613	GLU
1	B	620	MET
1	B	1010	ASN
1	B	1027	MET
1	B	1130	LYS
1	B	1161	PRO

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Mol	Chain	Res	Type
1	B	1228[A]	SER
1	B	1228[B]	SER
1	B	1259	ILE
1	B	1270	LYS
1	B	1275	GLU
1	B	1279	GLU
1	B	1346	ILE
1	B	1362	VAL
1	B	1408	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	GLN
1	A	616	GLN
1	A	1054	ASN
1	A	1324	GLN
1	A	1368	GLN
1	B	476	ASN
1	B	501	HIS
1	B	1081	HIS
1	B	1320	ASN
1	B	1324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	B	1502	-	4,4,4	0.31	0	6,6,6	0.06	0
4	SO4	B	1503	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	A	1504	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	B	1504	-	4,4,4	0.30	0	6,6,6	0.18	0
5	A1DMB	C	101	-	41,42,42	3.12	14 (34%)	54,60,60	3.97	27 (50%)
4	SO4	A	1503	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	A	1502	-	4,4,4	0.40	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1DMB	C	101	-	-	5/15/34/34	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	101	A1DMB	C16-C17	-10.79	1.13	1.36
5	C	101	A1DMB	C16-C15	-9.17	1.26	1.41
5	C	101	A1DMB	C17-C18	-6.93	1.24	1.39
5	C	101	A1DMB	O2-C18	4.92	1.43	1.35
5	C	101	A1DMB	N7-N6	4.63	1.39	1.32
5	C	101	A1DMB	O3-C25	-4.54	1.32	1.37
5	C	101	A1DMB	C4-C5	3.80	1.53	1.47
5	C	101	A1DMB	C7-N2	3.45	1.52	1.47
5	C	101	A1DMB	C6-C5	2.79	1.42	1.37
5	C	101	A1DMB	C15-N4	-2.73	1.32	1.37
5	C	101	A1DMB	C12-C20	-2.69	1.37	1.43
5	C	101	A1DMB	C14-N4	2.40	1.35	1.31
5	C	101	A1DMB	C18-N5	2.12	1.36	1.31
5	C	101	A1DMB	C23-C4	2.01	1.42	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	101	A1DMB	C16-C17-C18	10.48	130.36	117.84
5	C	101	A1DMB	C16-C15-C20	-9.27	107.94	119.55
5	C	101	A1DMB	C2-N1-C1	-8.27	114.55	124.45
5	C	101	A1DMB	C17-C16-C15	8.15	130.55	120.80
5	C	101	A1DMB	N2-N6-N7	7.89	113.76	107.09
5	C	101	A1DMB	C17-C18-N5	-7.58	111.20	125.11
5	C	101	A1DMB	O2-C18-C17	6.86	128.91	116.77
5	C	101	A1DMB	C6-N2-N6	-6.83	104.20	110.63
5	C	101	A1DMB	C16-C15-N4	6.04	128.28	118.55
5	C	101	A1DMB	O3-C25-C2	-5.98	116.65	120.74
5	C	101	A1DMB	C7-N2-C6	5.74	138.27	128.77
5	C	101	A1DMB	C5-C6-N2	5.31	110.38	105.31
5	C	101	A1DMB	C5-N7-N6	-5.25	103.60	109.23
5	C	101	A1DMB	O1-C1-N1	5.09	126.78	121.39
5	C	101	A1DMB	C22-C7-N2	4.35	116.91	110.95
5	C	101	A1DMB	C19-O2-C18	-3.48	112.15	117.33
5	C	101	A1DMB	C21-C22-C7	2.76	115.84	110.78
5	C	101	A1DMB	C9-C8-C7	2.70	115.72	110.78
5	C	101	A1DMB	C7-N2-N6	-2.53	117.50	120.94
5	C	101	A1DMB	O3-C25-C24	2.39	120.70	116.89
5	C	101	A1DMB	C4-C5-N7	2.37	125.86	122.05
5	C	101	A1DMB	C13-C12-C20	-2.35	114.52	117.96
5	C	101	A1DMB	C4-C5-C6	-2.33	126.09	129.65
5	C	101	A1DMB	C3-C2-N1	2.30	123.76	119.76
5	C	101	A1DMB	C10-C11-C12	2.29	117.33	112.51
5	C	101	A1DMB	F1-C13-C12	2.17	120.39	117.66
5	C	101	A1DMB	C14-N4-C15	-2.06	114.58	116.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

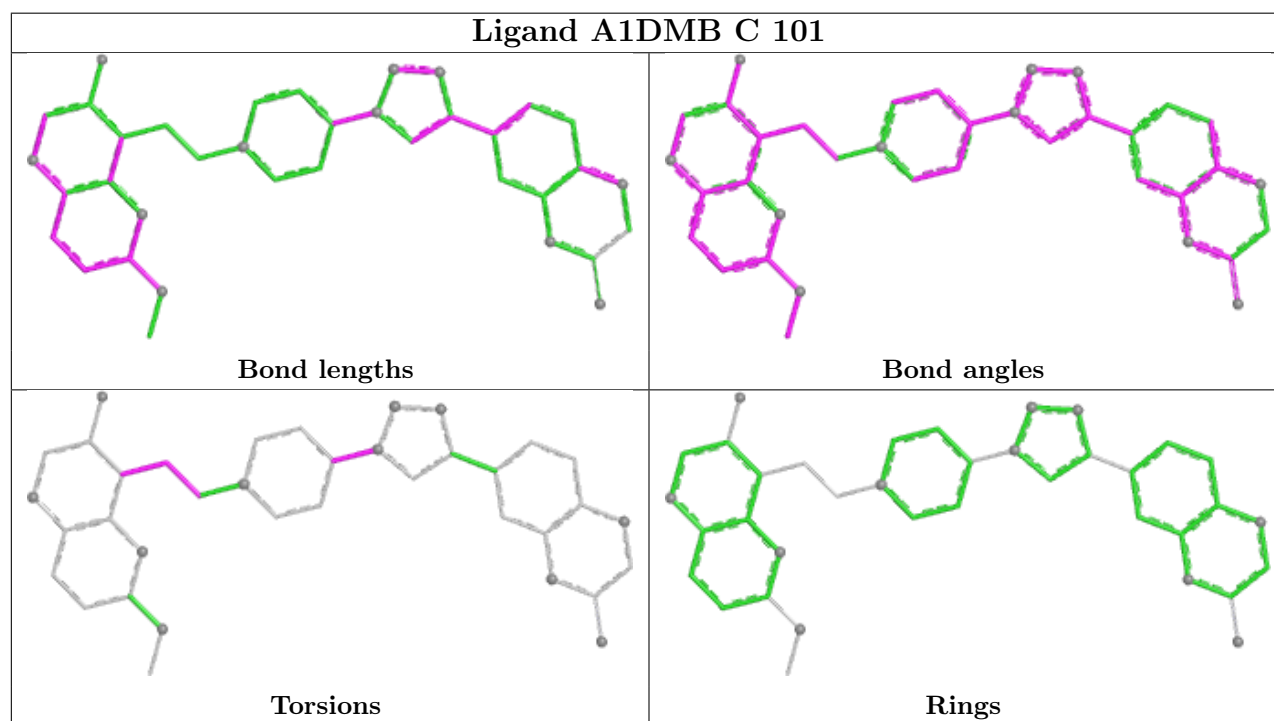
Mol	Chain	Res	Type	Atoms
5	C	101	A1DMB	C10-C11-C12-C13
5	C	101	A1DMB	C10-C11-C12-C20
5	C	101	A1DMB	N3-C10-C11-C12
5	C	101	A1DMB	C8-C7-N2-C6
5	C	101	A1DMB	C8-C7-N2-N6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1503	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	670/693 (96%)	0.44	29 (4%) 40 42	15, 33, 51, 78	3 (0%)
1	B	671/693 (96%)	0.46	25 (3%) 45 48	12, 33, 56, 80	3 (0%)
2	C	20/20 (100%)	-0.60	0 100 100	19, 27, 42, 44	0
2	D	20/20 (100%)	-0.44	0 100 100	19, 26, 60, 67	0
All	All	1381/1426 (96%)	0.42	54 (3%) 43 46	12, 33, 54, 80	6 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1490	LEU	5.8
1	A	1490	LEU	3.9
1	A	416	GLY	3.4
1	B	491	GLY	3.2
1	B	639	TYR	3.1
1	A	1436	LEU	3.1
1	A	490	GLY	3.0
1	B	1009	ILE	3.0
1	B	612	ILE	2.9
1	B	611	ALA	2.9
1	A	1449	LEU	2.9
1	B	487	THR	2.8
1	B	493	PHE	2.8
1	B	604	LEU	2.7
1	A	1092	ARG	2.7
1	A	1024	ASP	2.7
1	A	1439	ASP	2.7
1	B	1460	ALA	2.6
1	A	1448	LEU	2.5
1	A	638	VAL	2.5
1	A	1465	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	489	ILE	2.5
1	A	1415	PHE	2.4
1	B	625	VAL	2.4
1	A	1254	GLY	2.4
1	A	1481	GLY	2.4
1	B	417	LYS	2.4
1	A	1073	ASP	2.3
1	A	496	ALA	2.3
1	A	1443	ALA	2.3
1	B	638	VAL	2.3
1	A	1442	GLU	2.2
1	B	1056	GLN	2.2
1	B	467	ALA	2.2
1	B	482	ILE	2.2
1	A	424	LYS	2.2
1	B	496	ALA	2.2
1	B	614	ALA	2.2
1	A	1286	ILE	2.1
1	A	495	LEU	2.1
1	A	1299	ARG	2.1
1	B	1436	LEU	2.1
1	B	581	LYS	2.1
1	A	1278	ALA	2.1
1	A	491	GLY	2.1
1	A	1281	VAL	2.1
1	B	424	LYS	2.1
1	A	1287	ASP	2.1
1	A	1404	ASP	2.1
1	A	422	SER	2.1
1	B	468	ARG	2.1
1	B	1278	ALA	2.0
1	A	1440	LYS	2.0
1	B	1453	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

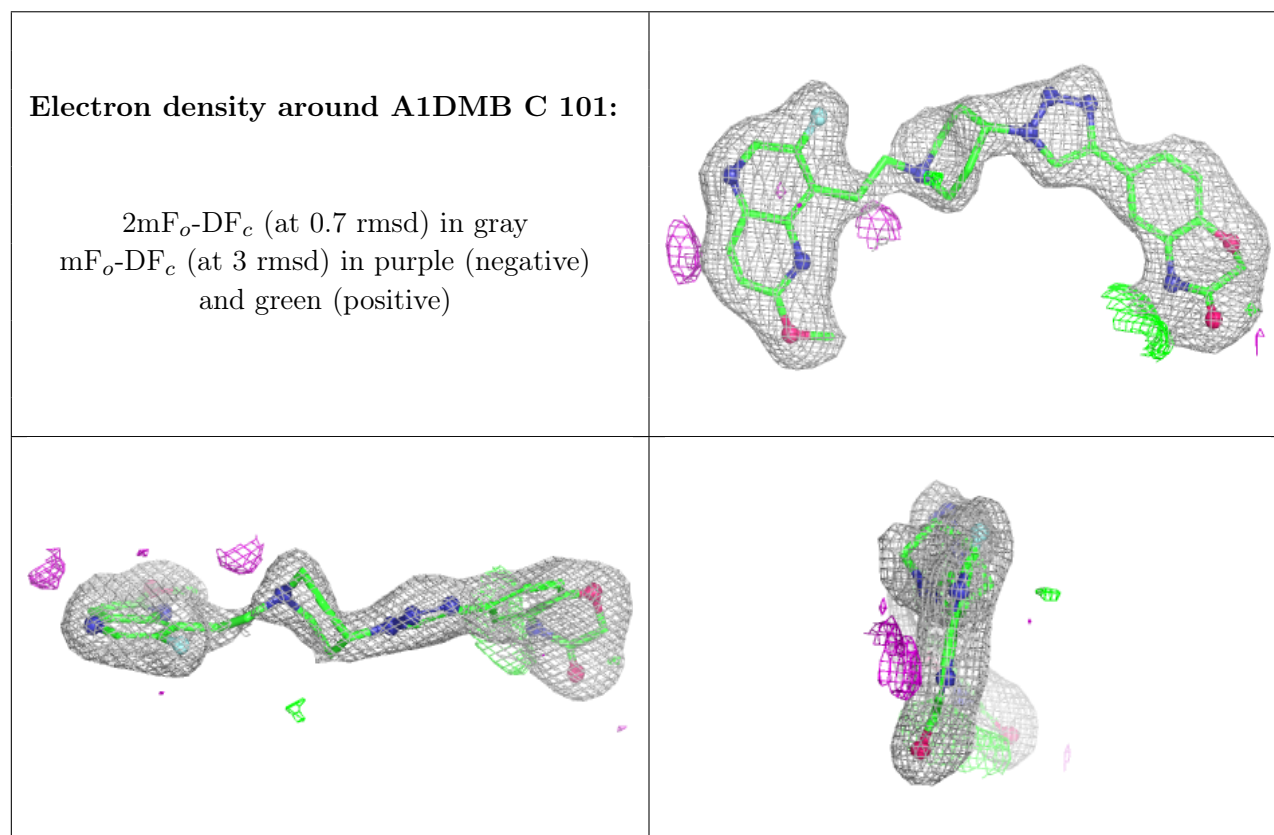
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	1504	5/5	0.75	0.13	85,104,107,108	0
4	SO4	A	1503	5/5	0.77	0.14	58,86,90,95	0
4	SO4	B	1503	5/5	0.80	0.13	50,55,63,68	0
4	SO4	B	1502	5/5	0.81	0.10	78,85,86,89	0
4	SO4	A	1502	5/5	0.88	0.14	32,47,63,70	0
4	SO4	B	1504	5/5	0.92	0.11	59,67,68,78	0
5	A1DMB	C	101	37/37	0.93	0.10	23,37,58,60	0
3	MN	A	1501	1/1	0.99	0.02	26,26,26,26	0
3	MN	B	1501	1/1	1.00	0.01	29,29,29,29	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.